IN: Yang, J.C., et al., Editors, Solid Propellant Gas Generators: Proceedings of the 1995 Workshop, NISTIR 5766, June 28-29, 1995, 89-122 pp, 1995

Modeling and Experimental Validation of Pyrotechnic Gas Generators

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NIST Gas Generator Workshop
Gaithersburg, MD

28 June, 1995

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BACKGROUND

- CONSULTANTS TO AIRBAG INDUSTRY
- MODELING WORK
    - developed general-purpose gas generator models
    - validated performance of numerous inflators
    - used in design of new inflators
- EXPERIMENTAL WORK
    - cold-flow test apparatus
    - combustion test apparatus
    - ignition test apparatus
    - design of experiments (DOE)
- ADVANCED CONCEPTS
    - next-generation inflator designs

AIRBAG COMPONENTS

- CRASH SENSORS AND COMPUTER LOGIC

- INFLATOR UNIT (i.e., both hybrid and pyrotechnic gas generators)
    - ignitor
    - propellant grains
    - hardware items
    - particle filter

- BAG HOLDER AND EXTERIOR PADDING

- NYLON AIRBAG ASSEMBLY

ENGINEERING CHALLENGES

- IGNITOR RELIABILITY (output history, is it repeatable ?)

- TIMING OF EVENTS (pressure-time profiles)

- PRODUCT CHEMICAL COMPOSITION
  - tank gas
  - tank particulates
  - inflator slag (multi-phase mixture)

- AMBIENT OPERATING ENVIRONMENT
  - temperature
  - pressure

- AIRBAG DEPLOYMENT
  - dynamics of bag filling
  - thermal and mechanical response of bag as it opens

- PROPELLANT LIFE (>15 years)

- PROPELLANT DISPOSAL

GOALS AND OBJECTIVES

- DEVELOP A MODEL THAT DESCRIBES THE THERMOCHEMICAL EVENTS OCCURRING IN A GAS GENERATOR

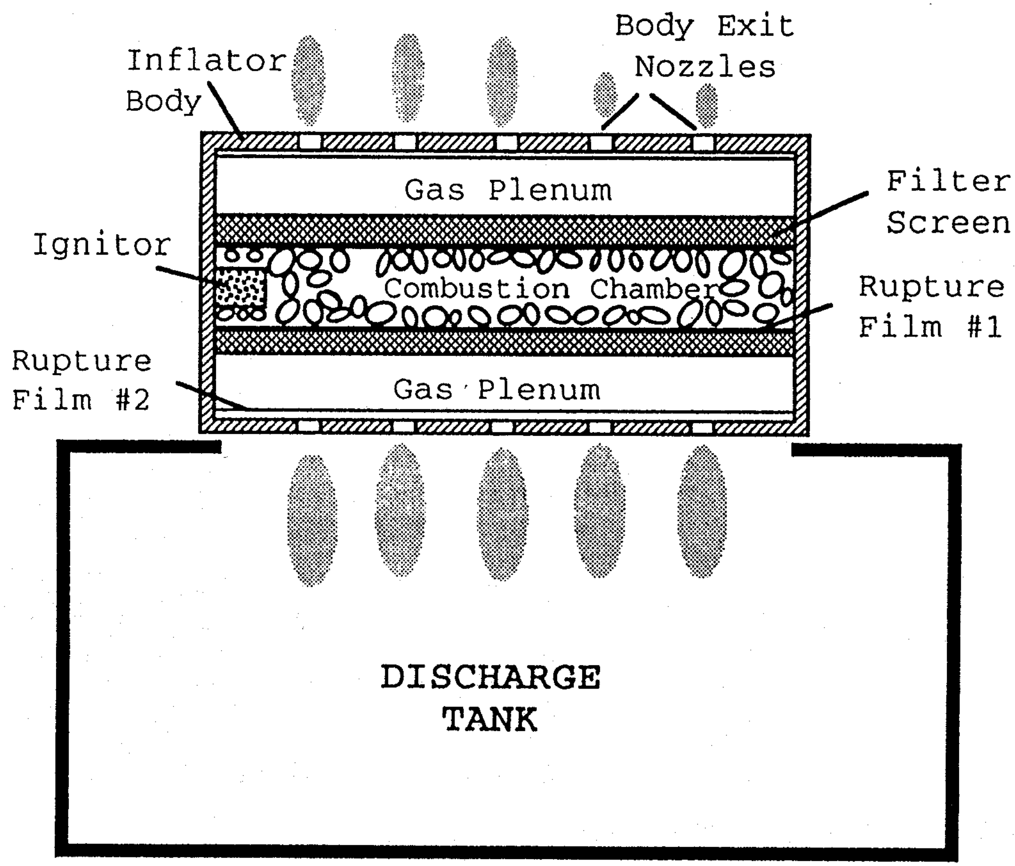
- VALIDATE MODEL WITH EXPERIMENTS

- STUDY THE INFLUENCE OF MATERIAL PROPERTIES AND DESIGN PARAMETERS ON PERFORMANCE OF GAS GENERATOR

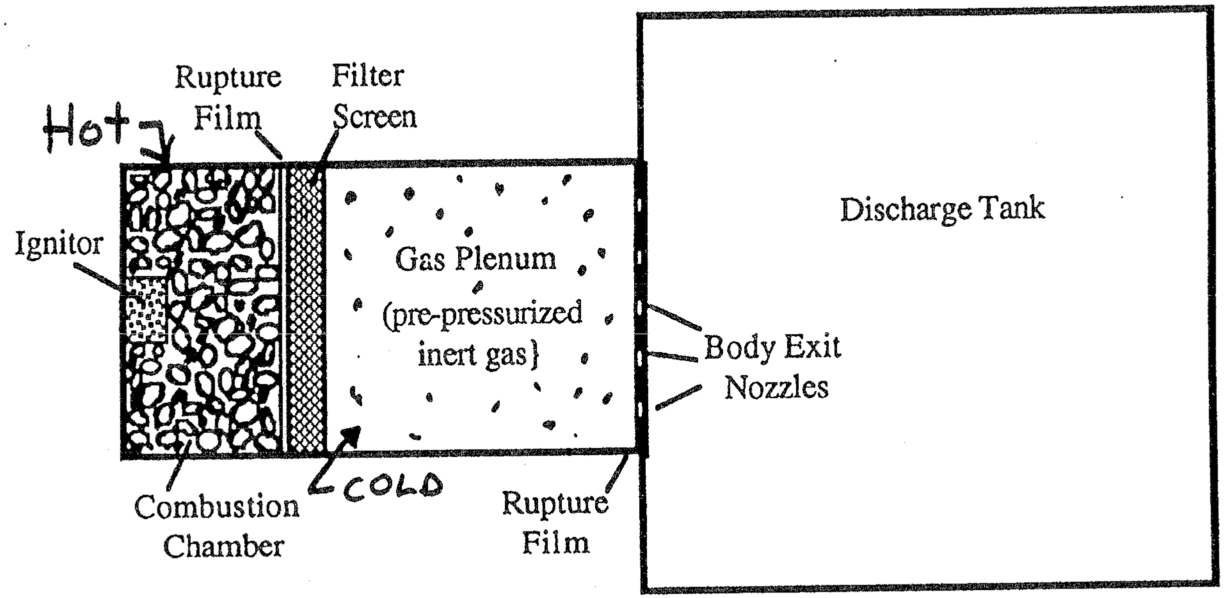
  - maximum inflator pressure, temperature
  - maximum tank pressure, temperature
  - tank impulse
  - pressure-time profiles
  - temperature-time profiles
  - tank gas composition

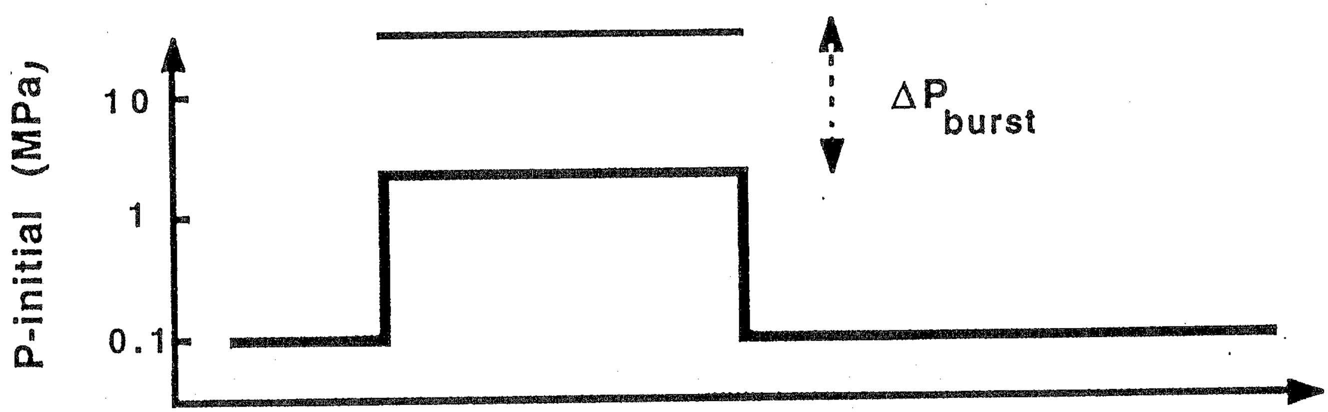
- COMPUTER PROGRAM FOR DESIGN OF NEW GAS GENERATORS

PHYSICAL MODEL
OF
GAS GENERATOR AND DISCHARGE TANK

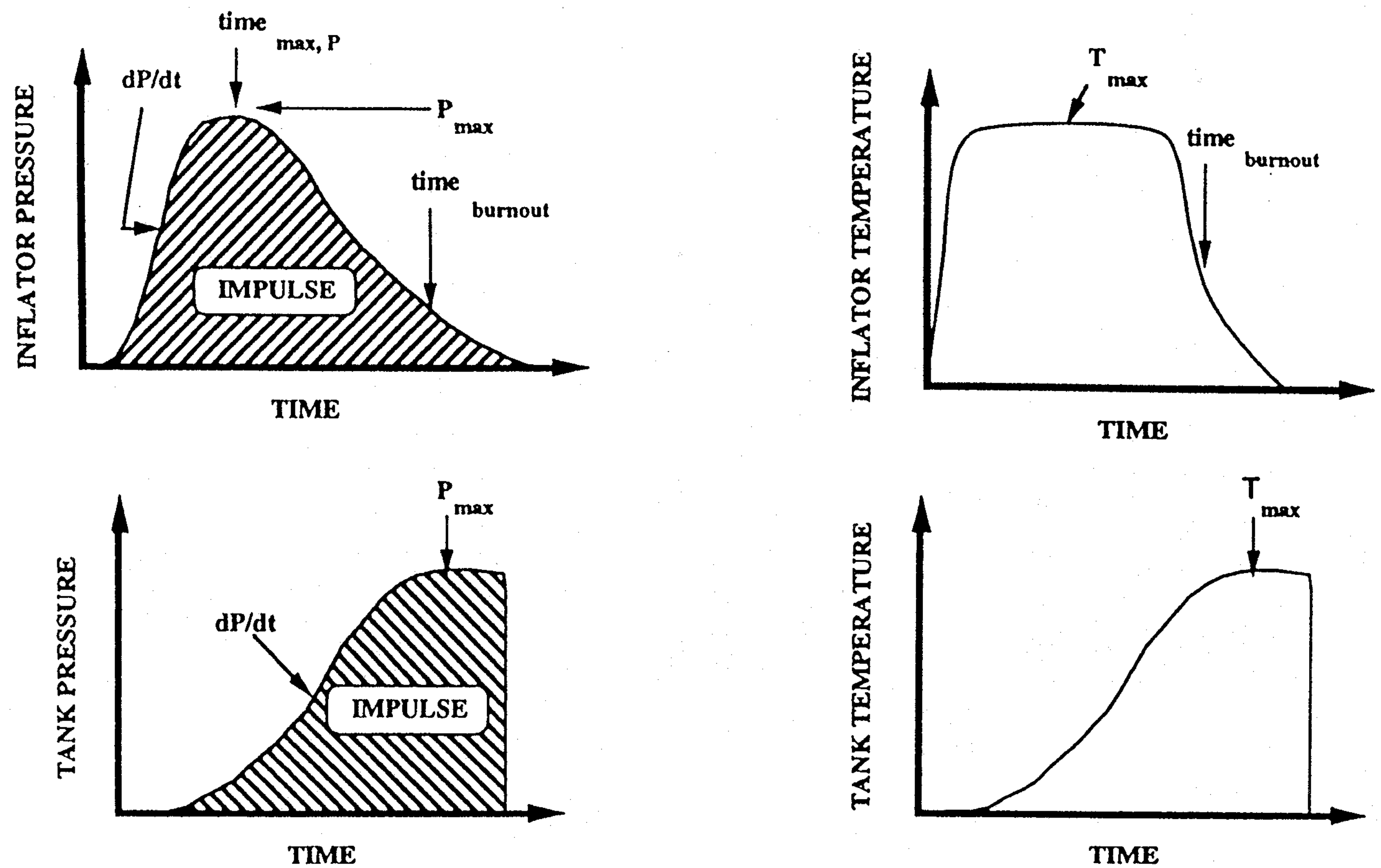


GAS-ASSISTED PYROTECHNIC INFLATOR





GAS GENERATOR PERFORMANCE PARAMETERS



COMPUTER SIMULATION

- **KEY FEATURES INCLUDED IN MODEL**
  - ignition time delay (flame spreading)
  - tracks individual species with time (g, s, l)
  - grain geometry (form function)
  - nozzle discharge flow rates
  - filter collection process and gas flow restriction

- **MODEL PREDICTING**
  - $P_J(t)$, $T_J(t)$, $X_J(t)$
  - heat exchange rates
  - hardware temperatures
  - propellant properties per time
  - flow properties at exit nozzle

- **EXPERIMENTAL VALIDATION DATA**
  - ignition delay time
  - mass of collected particles in filter
  - $P_J(t)$, $T_J(t)$, $X_{JJ}(t = \infty)$, $P_{JJ}(t = \infty)$

- **NUMERICAL PROCEDURE**
  - large system of ODE's (dT_i/dt, dm_K/dt, etc.)
  - solved using DVODE
  - CPU time is 0.1 - 1 minute on HP-735

MODEL DESCRIPTION

- BASED ON FUNDAMANTAL CONSERVATION LAWS (MASS, ENERGY)

- TWO MAJOR SUBSYSTEMS CONSIDERED:

  - gas generator assembly
  - discharge tank

- GAS GENERATOR ASSEMBLY INCLUDES:

  - body (metal hardware)
  - propellant grains
  - ignitor assembly
  - filter screen
  - thin metal foil for environmental seal and burst strength

- DISCHARGE TANK INCLUDES:

  - tank walls (heat loss)
  - mass discharged from inflator

- DIFFERENT MODES OF HEAT TRANSFER ARE CONSIDERED

MODEL ASSUMPTIONS

- FILTER <u>DOES NOT</u> COLLECT GAS SPECIES

- FILTER <u>DOES</u> COLLECT SOLID AND LIQUID PRODUCTS OF COMBUSTION

  - collection efficiency depends on filter design (mass, fiber size, etc.)

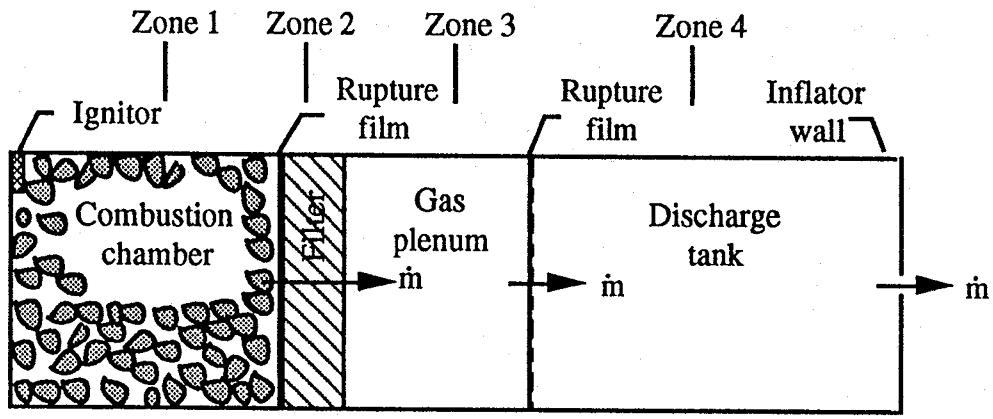
- GAS MIXTURE IS:

  - multiple species
  - $C_p(T)$
  - well-mixed, perfect gas
  - can be chemically reactive

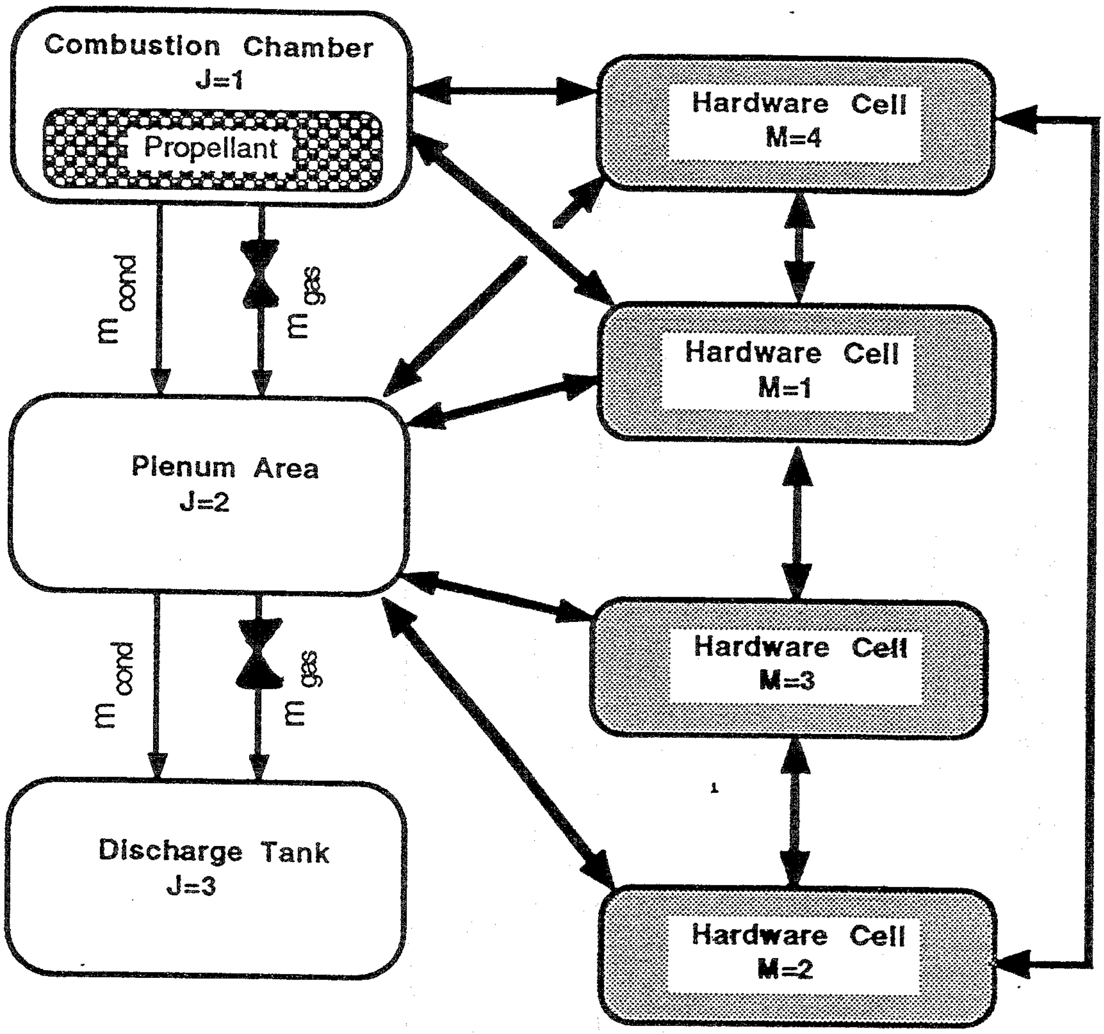
- CONDENSED SPECIES ARE:

  - multiple species
  - $C_p(T)$
  - not compressible

COMPUTATIONAL MODEL OF GAS GENERATOR AND DISCHARGE TANK



INFLATOR MODEL FLOW CHART

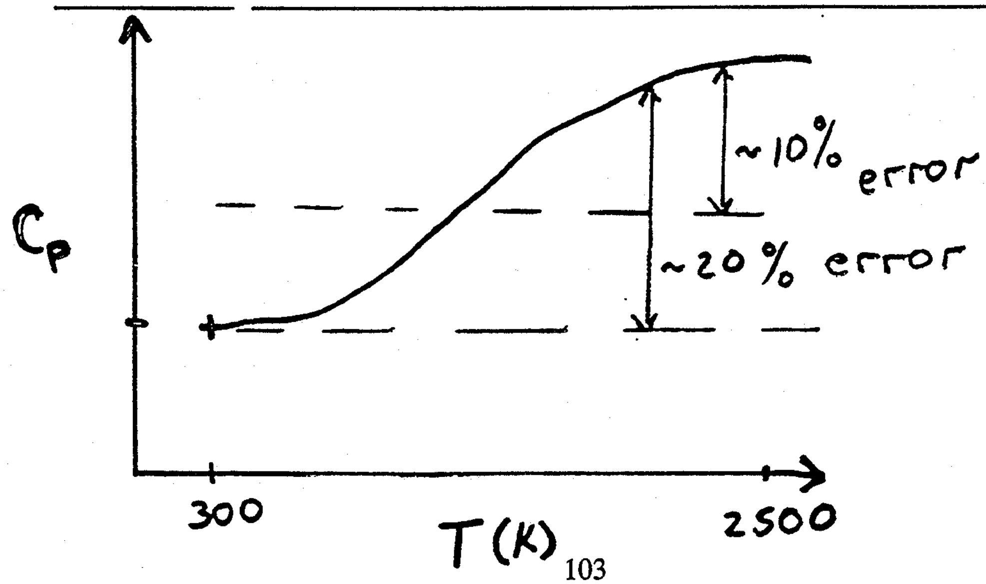


THERMODYNAMIC DATA BASE

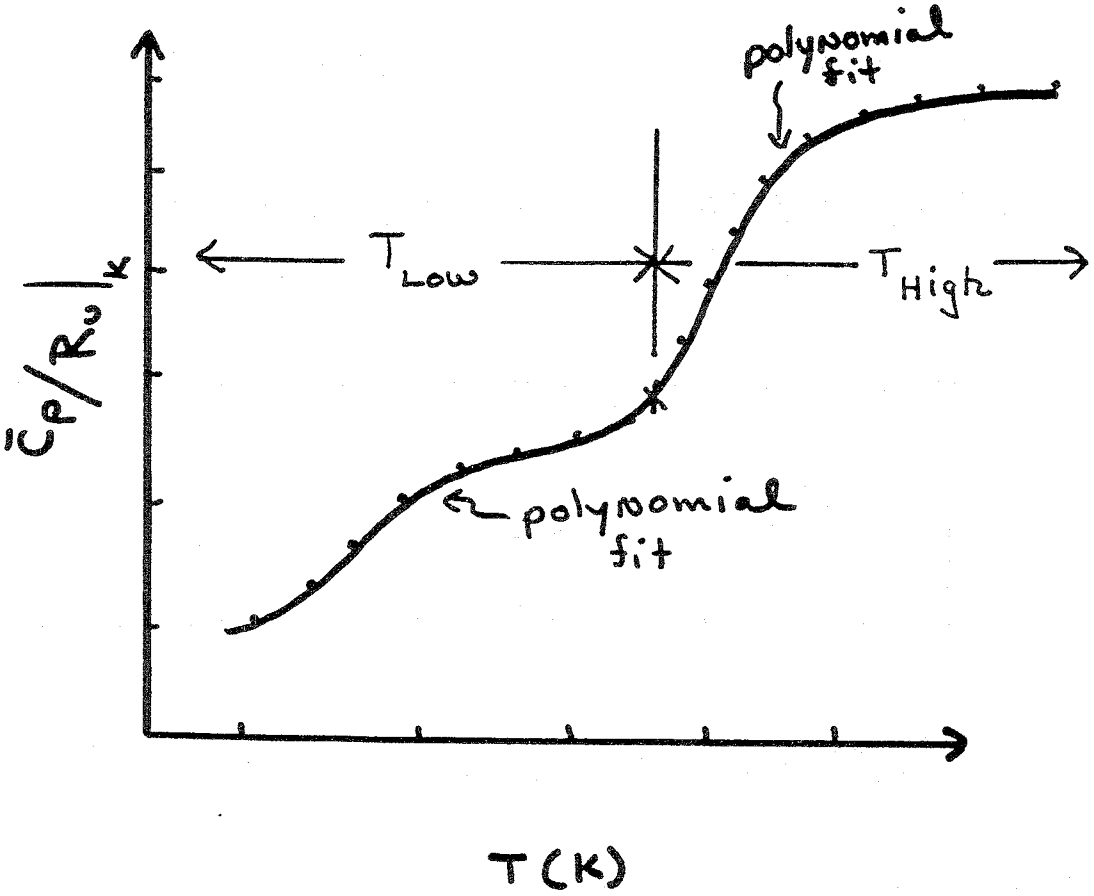
- Treats multiple chemical species in propellant grains and products of reaction
- Gaseous as well as condensed-phase species are possible
- Uses NASA/CHEMKIN thermodynamic data base for $C^o_{pk}(T)$

$$\boxed{\frac{C^o_{pk}(T)}{R} = a_{1k} + a_{2k}\,T + \ldots + a_{Nk}\,T^{(N-1)}}$$

- $C^o_{pk}(T)$ used to assemble enthalpy $H^o_k(T)$



SPECIFIC HEAT DATA



- gas $(300 < T(K) < 5000)$
- liquid $(T_M < T(K) < T_v)$
- solid (multiple phases) $(T < T_M)$
  - Debye temp.

GAS-PHASE CHEMISTRY

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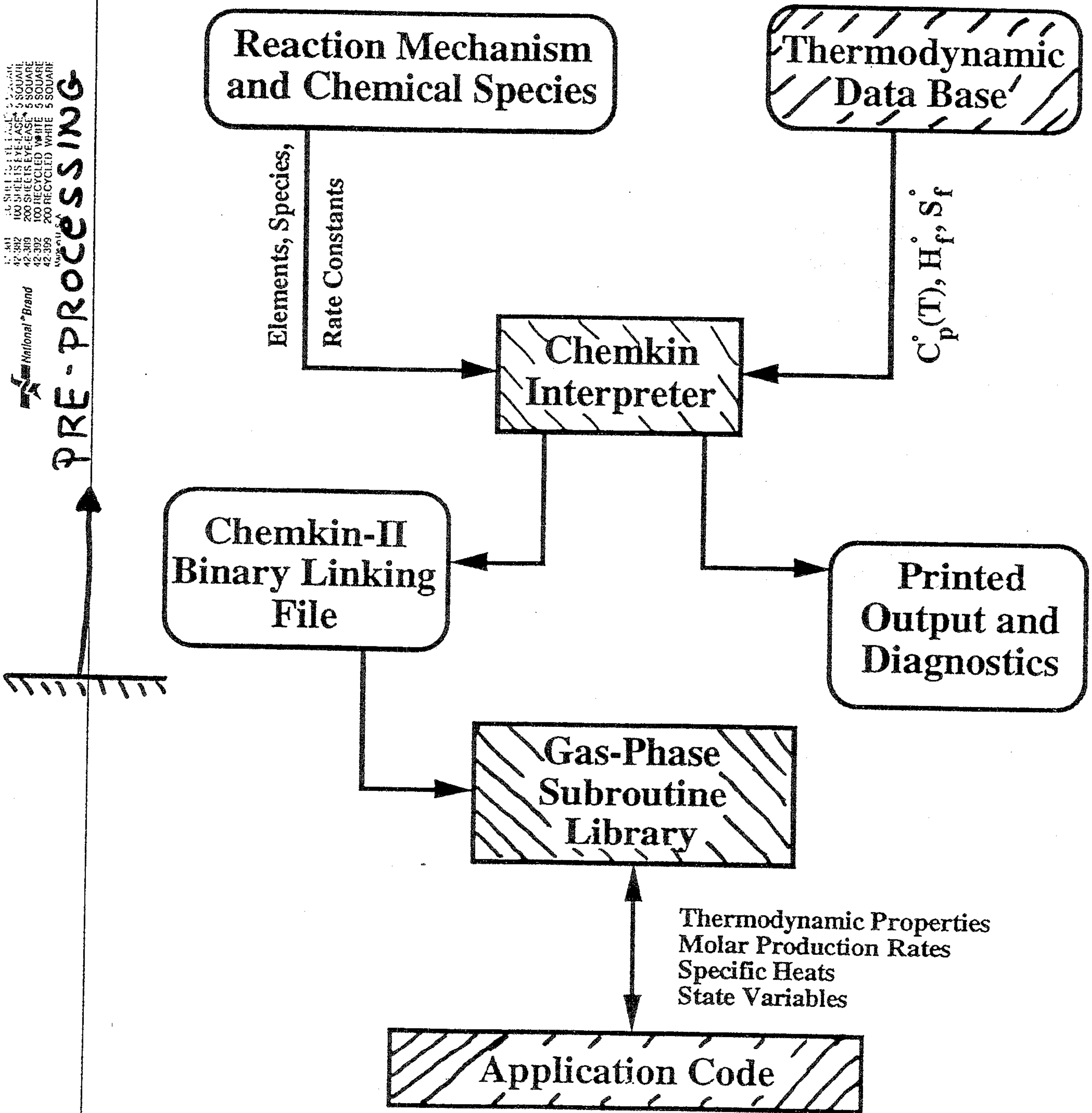
<<<<<<<  GAS-PHASE REACTIONS  >>>>>>>

Rxn number Symbolic representation
------------------------------------------------------------------------------
        1.    C+O2<=>CO+O
        2.    C+OH<=>CO+H
        3.    HCO+OH<=>H2O+CO
        4.    HCO+M<=>H+CO+M
        5.    HCO+H<=>CO+H2
        6.    HCO+O<=>CO+OH
        7.    HCO+O<=>CO2+H
        8.    HCO+O2<=>HO2+CO
        9.    CO+O+M<=>CO2+M
       10.    CO+OH<=>CO2+H
       11.    CO+O2<=>CO2+O
       12.    HO2+CO<=>CO2+OH
       13.    H2+O2<=>2OH
       14.    O+OH<=>O2+H
       15.    O+H2<=>OH+H
       16.    H+O2+M<=>HO2+M
```

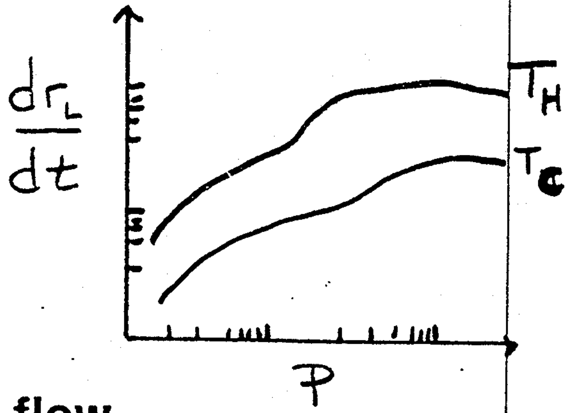
CHEMKIN-II: FLOW CHART



CONSTITUTIVE RELATIONS

- **Burn-rate**

$$\frac{dr_L}{dt} = b(T)\,\{a\,P^n\}$$

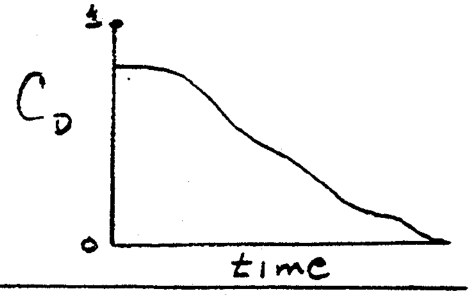


- **Flow at the exit ports is choked-flow**

$$\frac{dm_{ex}}{dt} = \frac{\Gamma\,A_{ex}\,P_i}{c_i} \times C_D \text{ (filter contamination)}$$

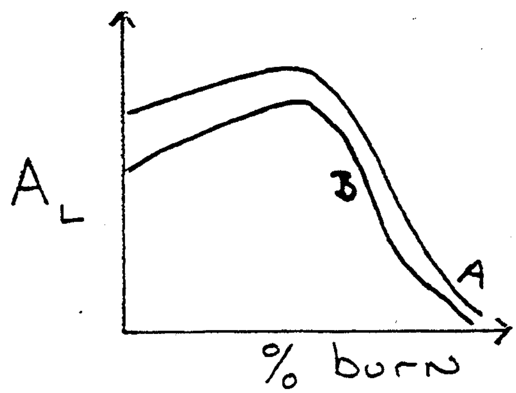
where Γ is a function of the specific heat ratio of the exit gas,

$$\Gamma = \gamma\left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma+1}{2(\gamma-1)}}$$



- **Instantaneous surface area (form function)**

$A_L(t)$ = function of grain geometry



PARTICLE FILTER

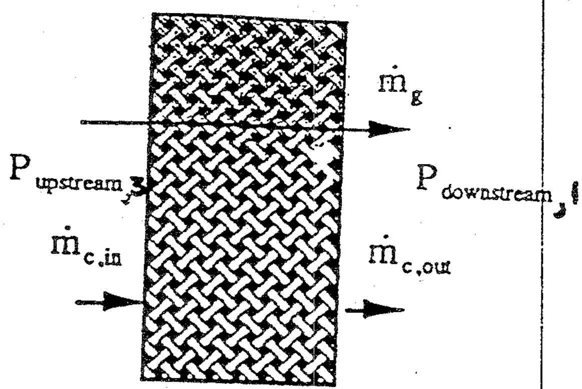
- **FILTER FLOW LOSS**

$$\dot{m}_{g,1,out} = \cancel{A}_{filter} C_{\mu,1} \left\{ \frac{2k}{k-1} P_1 \rho_1 \left[\left(\frac{P_3}{P_1}\right)^{\frac{2}{k}} - \left(\frac{P_3}{P_1}\right)^{\frac{k+1}{k}} \right] \right\}^{\frac{1}{2}}$$

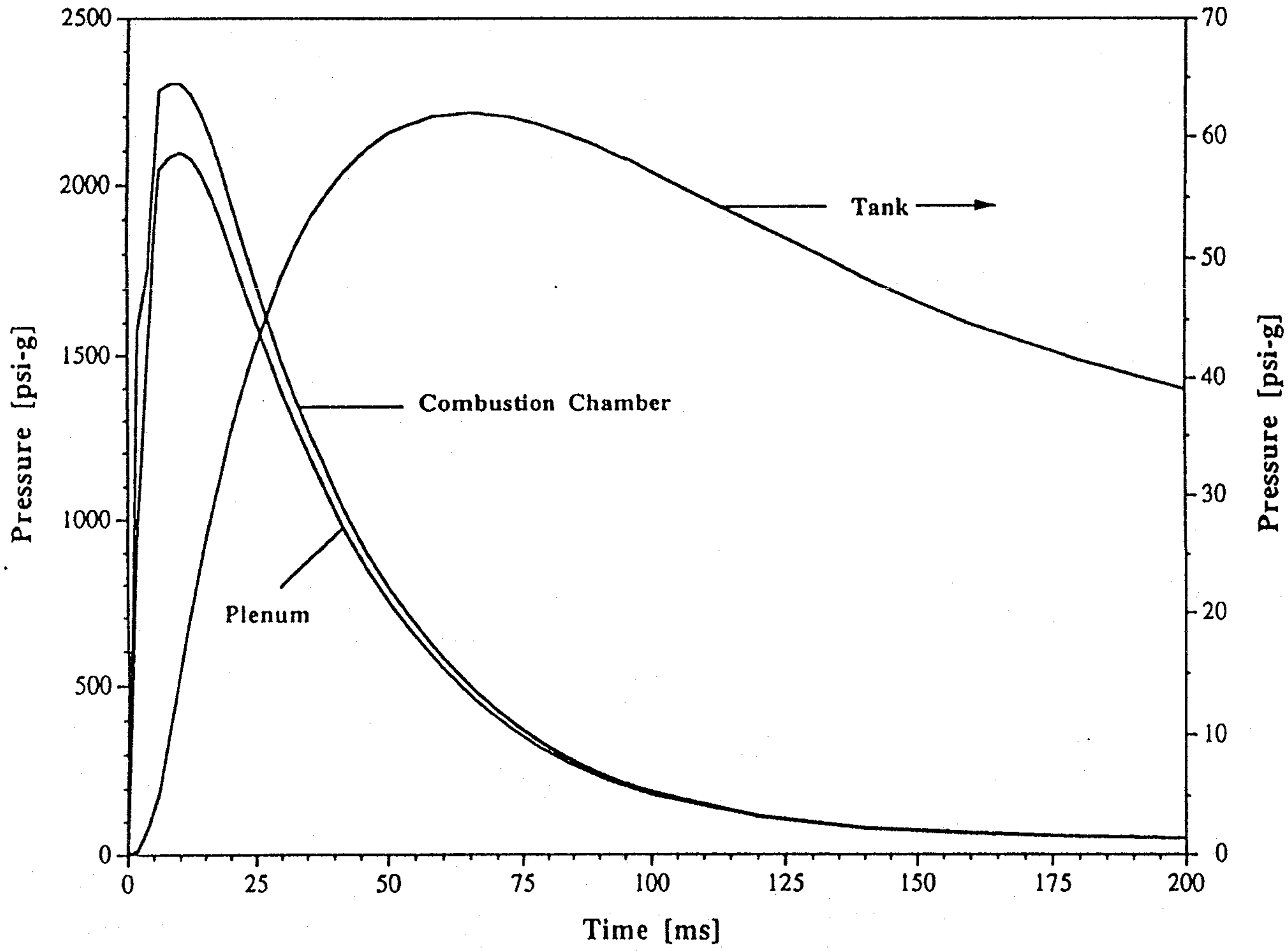
f(filter design)

- **FILTER COLLECTION EFFICIENCY**

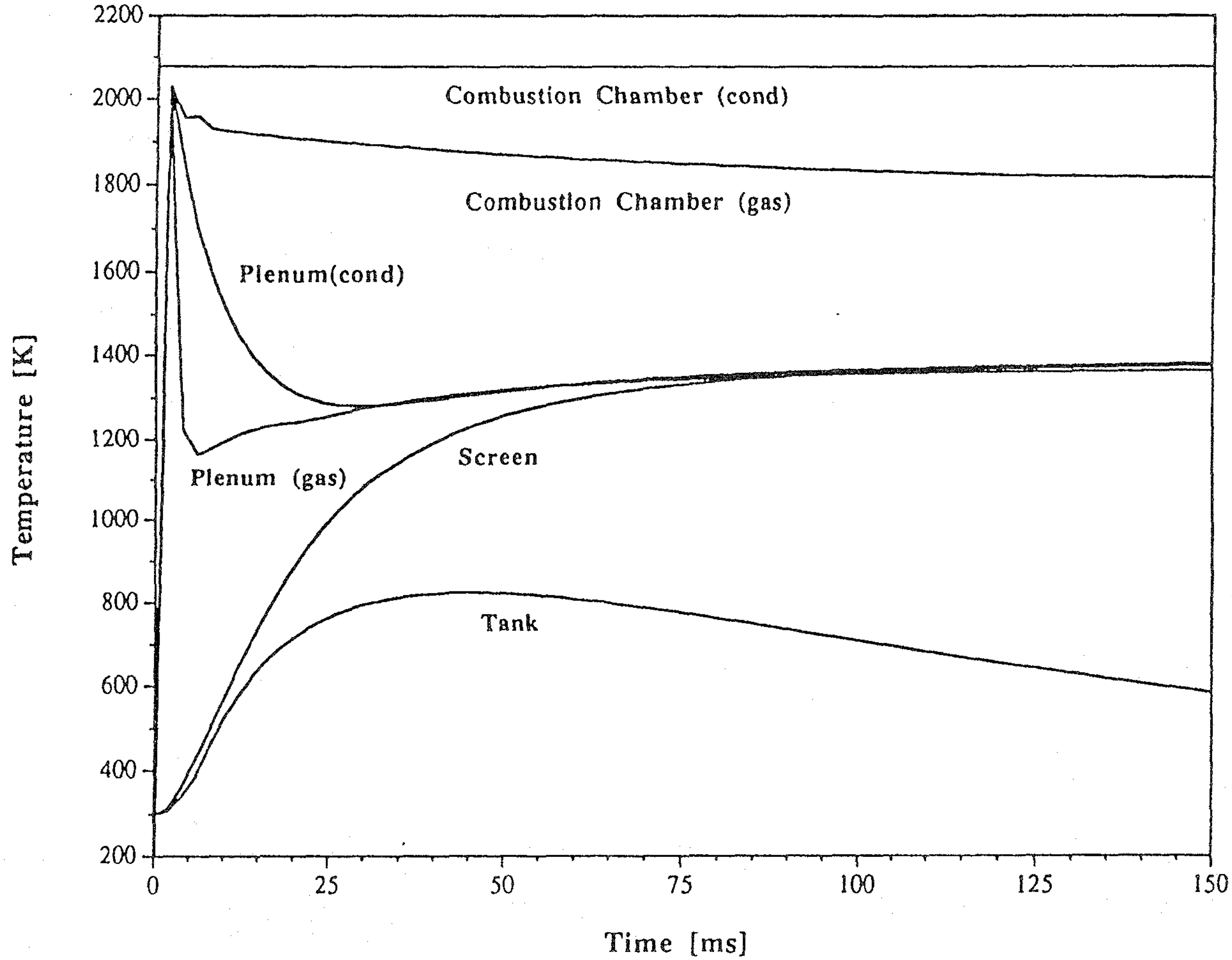
$$\dot{m}_{c,1,out} = \dot{m}_{g,1,out} \frac{m_{c,1}}{m_{g,1}}$$



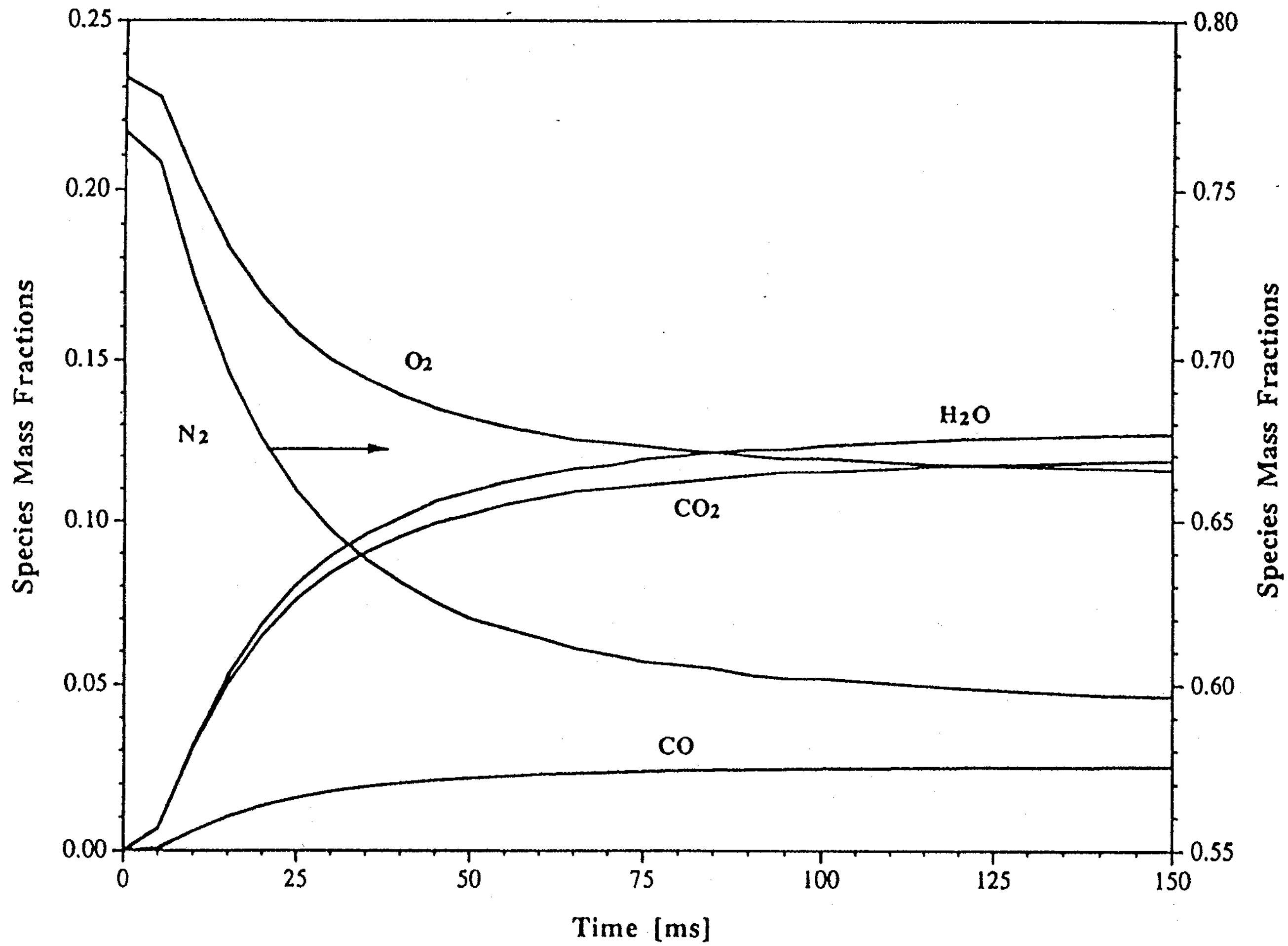
RESULTS - COMPUTER SIMULATION

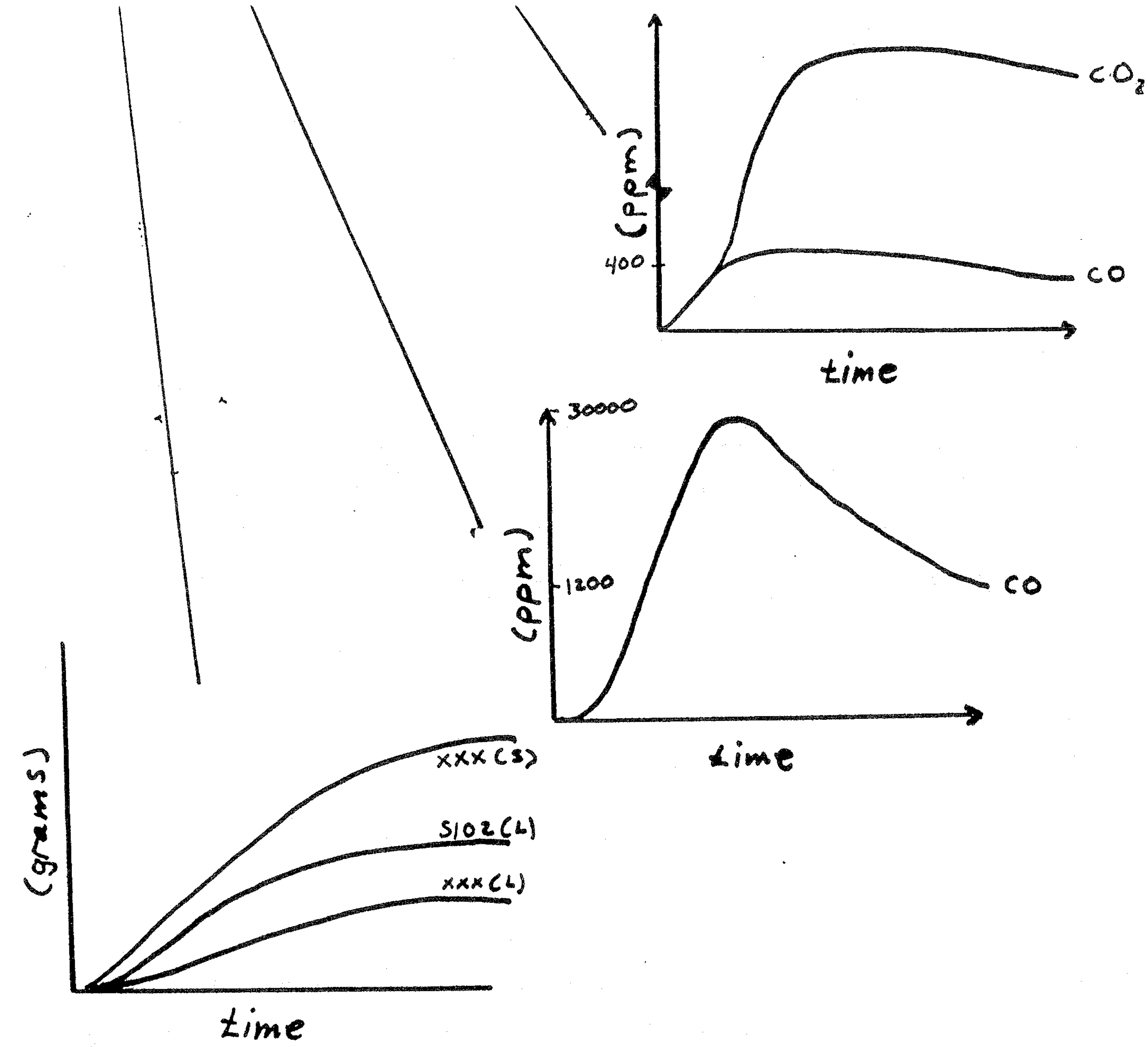


RESULTS - COMPUTER SIMULATION

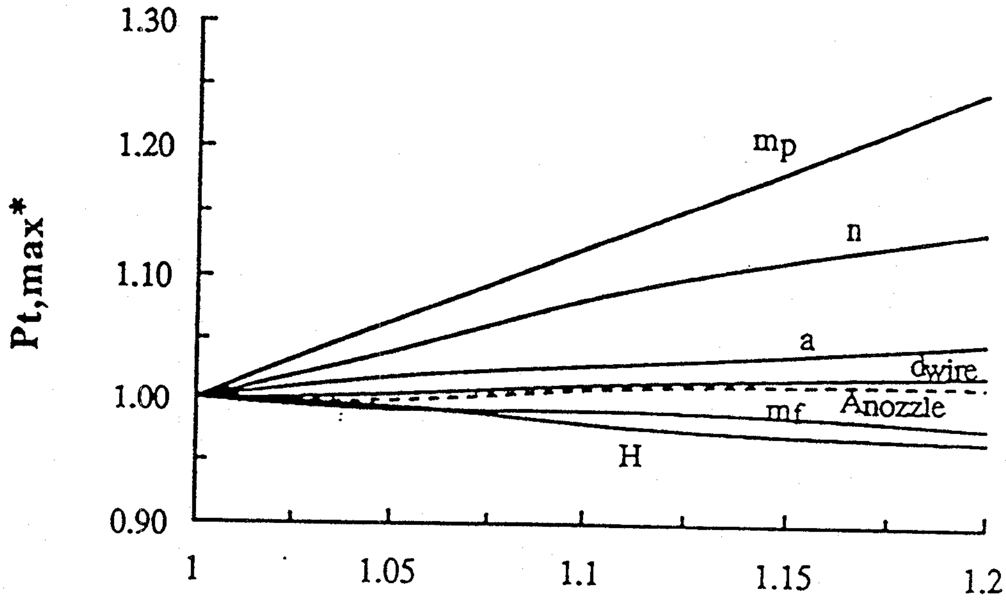


RESULTS - COMPUTER SIMULATION

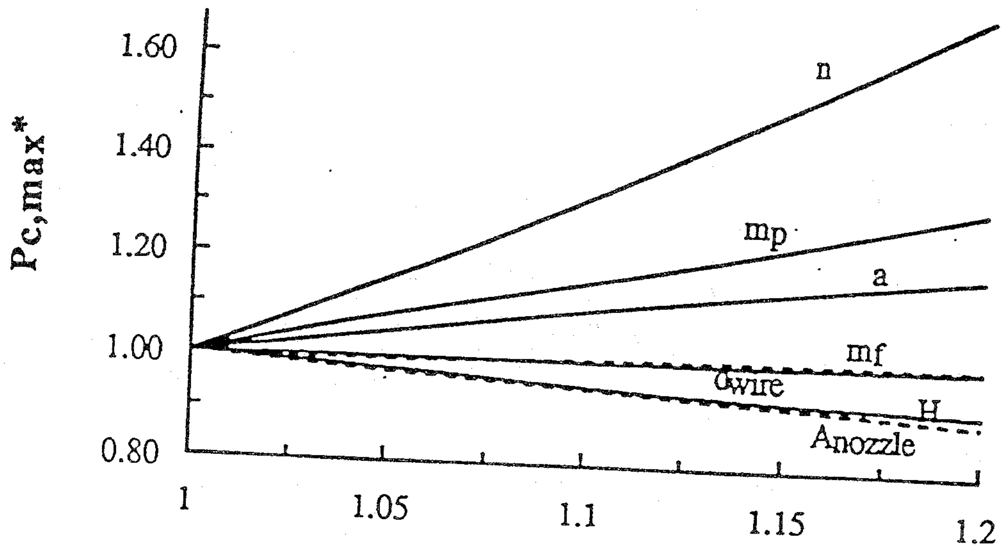



(ppm)
400
time
CO_2
CO
30000
1200
(ppm)
time
CO
(grams)
time
XXX (S)
SIO2 (L)
XXX (L)

RESULTS - SENSITIVITY STUDY



RESULTS - SENSITIVITY STUDY



NECESSARY FOR MEANINGFUL INFLATOR SIMULATION PROGRAM

- DESCRIPTION OF PROPELLANT AND PRODUCTS CHEMICAL COMPOSITION
- TEMPERATURE-DEPENDENT SPECIFIC HEAT FUNCTIONS FOR ALL POSSIBLE SPECIES
- PRECISE SOLID PHASE PROPERTIES (V, DENSITY)
- SURFACE REGRESSION RATE (= F(P,T))
- SURFACE/VOLUME RATIO OF PROPELLANT DURING BURN
- IGNITION SEQUENCE OF THE PROPELLANT (COATING, SQUIB SIZE, TEMPERATURE, ETC.)
- FRACTURE OF GRAINS DURING RAPID PRESSURIZATION
- SOLID-PHASE THERMAL PROPERTIES (MODEL SLAG FORMATION)
- NOZZLE OPENING PROCESS (INCLUDED MULTIPLE NOZZLE SIZES TO AVOID SADDLING EFFECT)
- HEAT LOSS TO SCREENS
- DYNAMIC MASS-FLOW DISCHARGE COEFFICIENTS
- DEVELOPMENT OF EXPERIMENTAL PLAN IN PARALLEL WITH MODEL DEVELOPMENT

EXPERIMENTAL REQUIREMENTS

- DESCRIPTION OF PROPELLANT
  - chemical composition
  - grain geometry
  - burn-rate function

- ANALYSIS OF SPECIES REMAINING IN THE INFLATOR AFTER FIRING

- DYNAMIC PRESSURE MEASUREMENTS IN:
  - inflator body
  - discharge tank

- AFTER-FIRING INSPECTION OF HARDWARE FOR CONDENSED PARTICLES

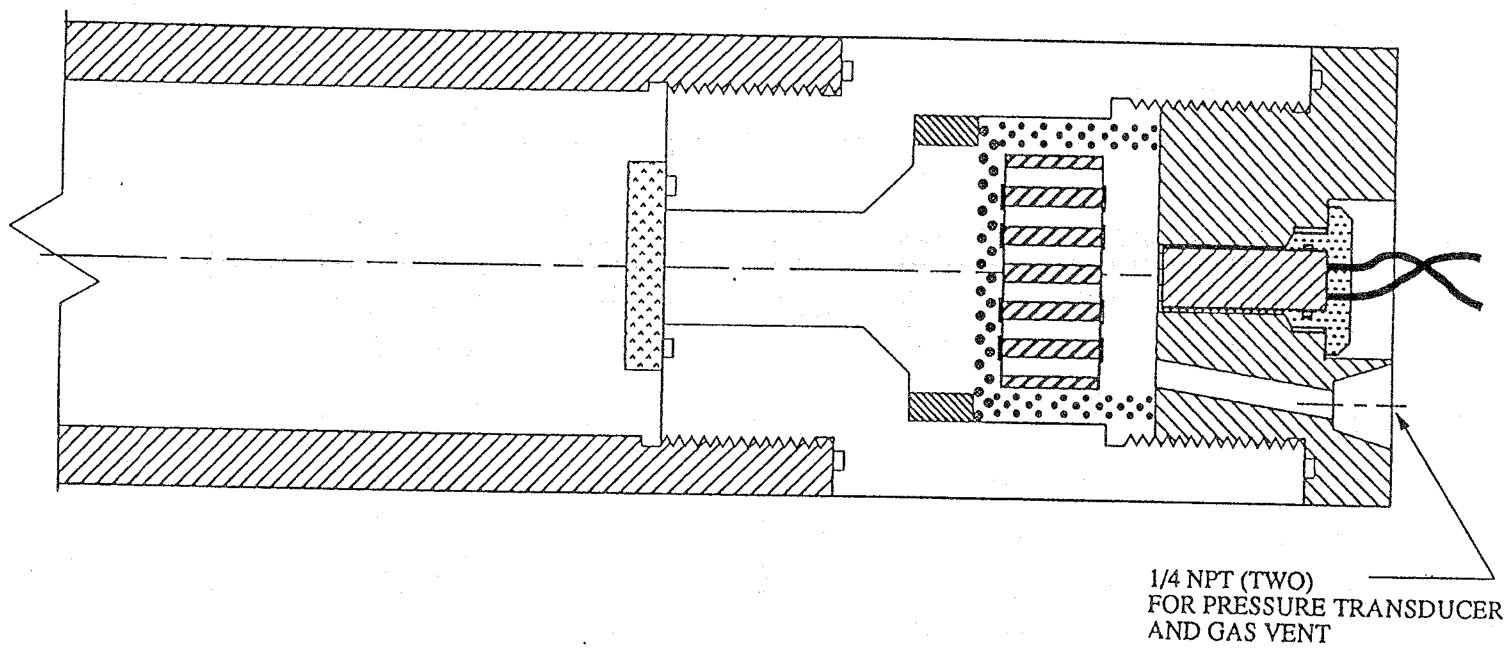
- INDEPENDENT STUDIES OF THE FILTER COLLECTION EFFICIENCY

- INDEPENDENT STUDIES OF THE PROPELLANT IGNITION SEQUENCE

PROPELLANT CONCERNS

- PRODUCT CHEMICAL COMPOSITION
  - tank gas
  - tank particulates
  - inflator slag (multi-phase mixture)
- LIFE (>15 years)
- DISPOSAL
- PROPELLANT OUTPUT
  - hot vs. cold firing
  - squib can fracture propellant grains
- LABORATORY COMBUSTION STUDIES SHOULD REPLICATE ACTUAL GAS GENERATOR OPERATING ENVIRONMENT
  - high confinement (solids loading)
  - pressure variations (14.7 - 4,000 psi)
  - possible slag build-up
  - flame spreading

COMBUSTION TEST APPARATUS



IGNITION CONCERNS

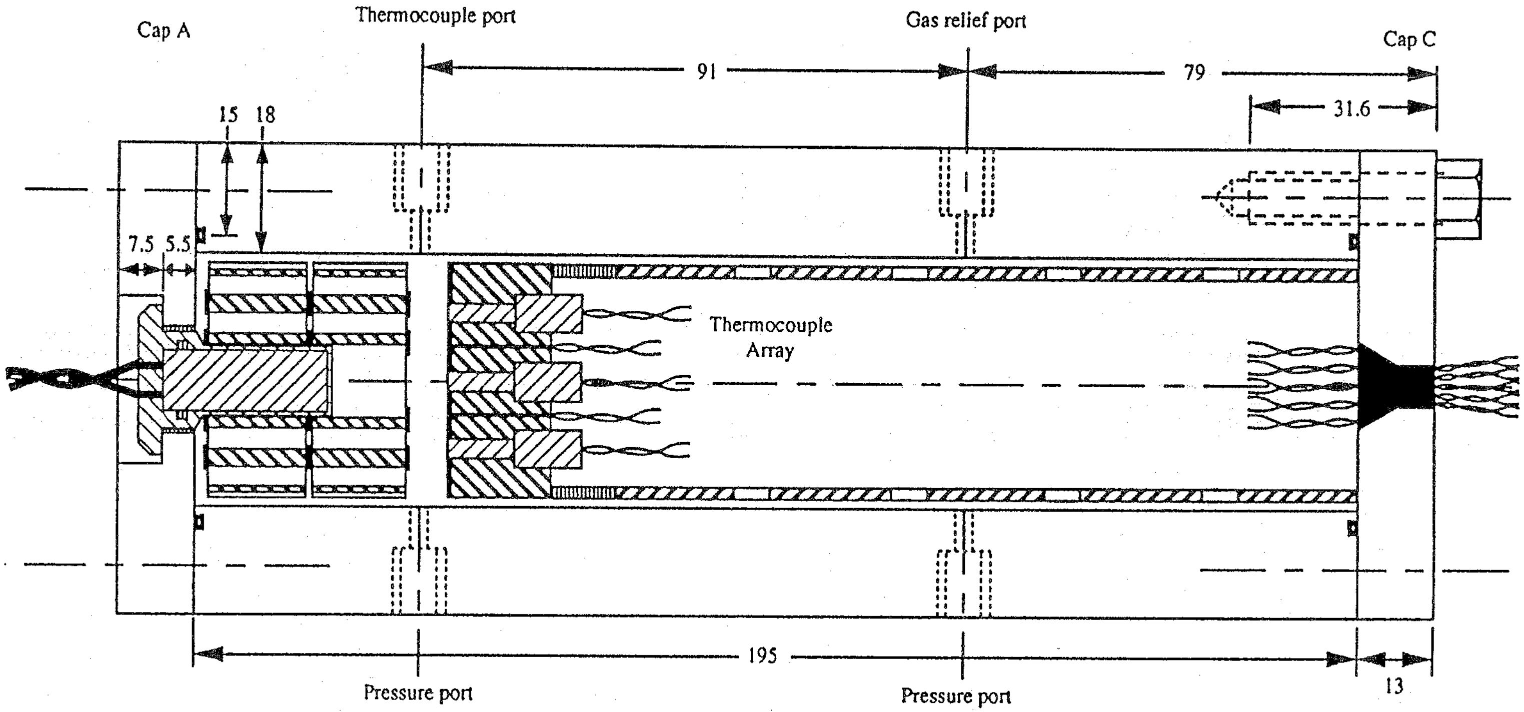
- **ACTION TIME**
  - hot vs. cold firing
  - uniform performance of "similar" squibs
  - some "good" gas-generating propellants require accelerant coatings

- **IGNITOR OUTPUT**
  - hot vs. cold firing
  - uniformity in performance of "similar" squibs
  - can fracture propellant grains

- **IGNITOR LIFE**
  - uniform performance after storage

- **INDEPENDENT STUDIES OF IGNITOR AND PROPELLANT IGNITION SEQUENCE ARE NECESSARY UNDER ALL OPERATING CONDITIONS**

IGNITION TEST APPARATUS



CONCLUSIONS

- COMPREHENSIVE GAS GENERATOR MODEL WAS DEVELOPED

- MODEL HAS BEEN APPLIED TO

  - conventional pyrotechnic inflators
  - hybrid inflators

- AGREEMENT WITH DATA IS EXCELLENT

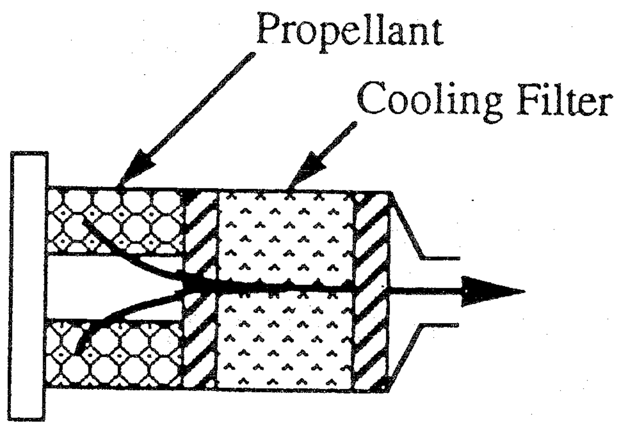
- MODEL IS A USEFUL TOOL FOR DESIGN AND DEVELOPMENT OF:

  - new inflators (material properties, size, etc.)
  - new pyrotechnic compositions
  - propellant grain modifications
  - ignitors
  - new filter designs

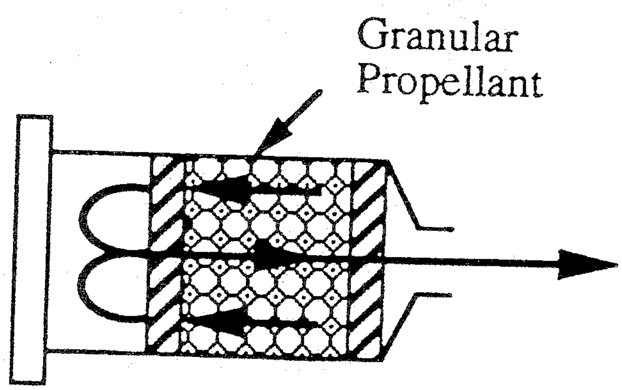
- EXPERIENCE SHOWS THAT A RELIABLE EXPERIMENTAL DATABASE IS ESSENTIAL

- WE RECOMMEND THAT SOLID PROPELLANT FIRE EXTINGUISHMENT PROGRAM FOLLOW SAME METHODOLOGY

ALTERNATIVE DESIGNS



a.) Standard Scheme



b.) Self-cooling Scheme